

OPTIMAL ACCELERATION OF CONVERGENCE*

ARIEH ISERLES[†] AND XIAOYAN LIU[‡]

Abstract. In this paper we investigate the *quadratic model*

$$\frac{\mathbf{b}^T \mathbf{u} + \mathbf{u}^T C \mathbf{u}}{\mathbf{a}^T \mathbf{u}},$$

which generalises the Shanks transformation and the familiar Padé model, to accelerate the convergence of a sequence $\{u_k\}_{k \in \mathbb{Z}^+}$. In the new model,

$$\mathbf{u}^T = [u_0, u_1, \dots, u_n],$$

$\mathbf{a}, \mathbf{b} \in \mathbb{R}^{n+1}$ and C is an $(n+1) \times (n+1)$ Hermitian matrix. (Note that, although \mathbf{u} might be complex, we use the transpose \mathbf{u}^T , rather than the adjoint \mathbf{u}^* .) Let us assume that the original sequence is obtained from the dynamical system $z \mapsto f(z)$, where $f(z) = \hat{u} + \sum_{k=1}^{\infty} \frac{1}{k!} \beta_k (z - \hat{u})^k$ is analytic about its fixed point $\hat{u} \in \mathbb{C}$. Suppose that $u_0 = \hat{u} + \varepsilon$ and $u_k = f^{\circ k}(u_0)$. It is easy to show that $\mathbf{b} = \mathbf{0}$ and $\mathbf{a} = 2C\mathbf{1}$. We give an iterative formula for the construction of the matrices C . Furthermore, we discuss the rate of convergence, inclusive of the special case when the fixed point is at ∞ .

1. The quadratic model. The starting point for the Shanks transformation is that, given a sequence $\{u_k\}_{k \in \mathbb{Z}^+}$, we construct the function

$$G(z) := u_0 + \sum_{k=1}^{\infty} (u_k - u_{k-1}) z^k$$

and take the $[N/N]$ Padé approximant to F at $z = 1$ as the ‘accelerated’ limit [1].

Its obvious generalisation is to consider

$$G(z) = \sum_{m=0}^{\infty} \left[\sum_{j=0}^m (-1)^{m-j} \alpha_{m,j} u_j \right] z^m$$

and its sections

$$G^{[n]}(z) = \sum_{m=0}^n \left[\sum_{j=0}^m (-1)^{m-j} \alpha_{m,j} u_j \right] z^m.$$

Having fixed n , we stipulate that $G^{[n]}(1) = u_n$. Thus,

$$\sum_{j=0}^n \left[\sum_{m=j}^n (-1)^{m-j} \alpha_{m,j} \right] u_j = u_n$$

and, since we want the coefficients to be independent of $\{u_k\}_{k \in \mathbb{Z}^+}$, we stipulate $\alpha_{n,n} = 1$ and

$$(1.1) \quad \sum_{m=j}^n (-1)^{m-j} \alpha_{m,j} = 0, \quad j = 0, 1, \dots, n-1.$$

*Received Sept. 27, 1999; revised April 10, 2001.

[†]Department of Applied Mathematics and Theoretical Physics, University of Cambridge, England (A.Iserles@damtp.cam.ac.uk).

[‡]Department of Mathematics and Physics, University of La Verne, USA (liux@ULV.EDU).

This is our first model, and we call it the *Padé model*.

Another general scheme for convergence acceleration is by letting the accelerator be

$$(1.2) \quad \frac{\mathbf{b}^T \mathbf{u} + \mathbf{u}^T C \mathbf{u}}{\mathbf{a}^T \mathbf{u}},$$

where

$$\mathbf{u}^T = [u_0, u_1, \dots, u_n]$$

$\mathbf{a}, \mathbf{b} \in \mathbb{R}^{n+1}$ and C is an $(n+1) \times (n+1)$ Hermitian matrix. Note that, although \mathbf{u} might be complex, we use the transpose \mathbf{u}^T , rather than the adjoint \mathbf{u}^* . We call this the *quadratic model*.

2. The quadratic model. Let us assume that the original sequence is obtained from the dynamical system $z \mapsto f(z)$, where $f(z) = \hat{u} + \sum_{k=1}^{\infty} \frac{1}{k!} \beta_k (z - \hat{u})^k$ is analytic about its fixed point $\hat{u} \in \mathbb{C}$. Suppose that $u_0 = \hat{u} + \varepsilon$. Then, expanding into series,

$$\begin{aligned} u_1 &= \hat{u} + \beta_1 \varepsilon + \frac{1}{2} \beta_2 \varepsilon^2 + O(\varepsilon^3), \\ u_2 &= \hat{u} + \beta_1^2 \varepsilon + \frac{1}{2} (\beta_1 + \beta_1^2) \beta_2 \varepsilon^2 + O(\varepsilon^3). \end{aligned}$$

Generally, we have (except when $\beta_1 = 1$)

$$(2.1) \quad u_k = f^{\circ k}(\hat{u} + \varepsilon) = \hat{u} + \beta_1^k \varepsilon + \frac{1}{2} \beta_1^{k-1} \frac{1 - \beta_1^k}{1 - \beta_1} \beta_2 \varepsilon^2 + O(\varepsilon^3), \quad k \in \mathbb{Z}^+,$$

where $f^{\circ k}$ is the k th iterate of the function f . Set

$$V(\varepsilon) = \frac{\mathbf{b}^T \mathbf{u} + \mathbf{u}^T C \mathbf{u}}{\mathbf{a}^T \mathbf{u}}.$$

The *order* of convergence acceleration (equivalently, the order of superattractivity at the fixed point) is the integer p such that

$$V(\varepsilon) = \hat{u} + O(\varepsilon^{p+1}).$$

The condition for $p \geq 0$ is that $V(0) = \hat{u}$. Let

$$\mathbf{p}_\ell := [1, \beta_1^\ell, \beta_1^{2\ell}, \dots, \beta_1^{n\ell}]^T, \quad \ell \in \mathbb{Z}^+$$

(for convenience, $\mathbf{p}_0 = \mathbf{1}$).

The ε^0 condition is

$$\mathbf{b}^T \mathbf{1} \hat{u} + \mathbf{1}^T C \mathbf{1} \hat{u}^2 = \mathbf{a}^T \mathbf{1} \hat{u}^2,$$

and we deduce that

$$(2.2) \quad \mathbf{b}^T \mathbf{1} = 0, \quad \mathbf{1}^T C \mathbf{1} = \mathbf{a}^T \mathbf{1}.$$

We turn our attention next to the ε condition: it is

$$\mathbf{b}^T \mathbf{p}_1 + 2 \mathbf{1}^T C \mathbf{p}_1 \hat{u} = \mathbf{a}^T \mathbf{p}_1 \hat{u}.$$

We first deduce that $\mathbf{b}^T \mathbf{p}_1 = 0$, and this implies $\mathbf{b} = \mathbf{0}$. Hence, no need to elaborate or mention any further that vector. More interesting consequence of equating powers of β_1 is

$$(2.3) \quad \mathbf{a} = 2C\mathbf{1}.$$

Comparing with (2.2), we deduce that

$$(2.4) \quad \mathbf{1}^T C\mathbf{1} = \mathbf{a}^T \mathbf{1} = 0.$$

Thus, we need to go further, considering the ε^2 terms, to argue that $p \geq 1$. This gives (for $\beta_1 \neq 0$ – otherwise the analysis is even simpler!)

$$\mathbf{p}_1^T C\mathbf{p}_1 + \hat{u} \frac{\beta_2}{\beta_1(1-\beta_1)} (\mathbf{p}_1 - \mathbf{p}_2)^T C\mathbf{1} = \frac{1}{2} \hat{u} \frac{\beta_2}{\beta_1(1-\beta_1)} (\mathbf{p}_1 - \mathbf{p}_2)^T \mathbf{a}$$

and (2.3) means that the $p \geq 1$ condition is just

$$(2.5) \quad \mathbf{q}^T C\mathbf{q} \equiv 0 \quad \text{for all} \quad \mathbf{q} = [1, q, q^2, \dots, q^n]^T, \quad q \in \mathbb{R}.$$

Hence

$$\sum_{k=0}^n \sum_{\ell=0}^n c_{k,\ell} q^{k+\ell} = 0, \quad q \in \mathbb{R},$$

and (2.5) can be alternatively expressed as

$$(2.6) \quad \begin{aligned} \sum_{k=0}^{\ell} c_{k,\ell-k} &= 0, & \ell &= 0, 1, \dots, n; \\ \sum_{k=\ell-n}^n c_{k,\ell-k} &= 0, & \ell &= n+1, \dots, 2n. \end{aligned}$$

Note, incidentally, that $\mathbf{1}^T C\mathbf{1} = 0$ is a special case of (2.5) when $q = 1$.

Recall from [2] that there exist numbers $\{\alpha_{m,\ell} : \ell = 1, \dots, m; m = 1, 2, \dots\}$ such that

$$f^{\circ k}(z) = \hat{u} + \sum_{m=1}^{\infty} \left(\sum_{\ell=1}^m \alpha_{m,\ell} \beta_1^{k\ell} \right) \varepsilon^m$$

(we exclude the cases of $\beta_1 = 0$ and of β_1 being a root of unity). Consequently, and exploiting $\mathbf{1}^T C\mathbf{1} = 0$, we obtain

$$(2.7) \quad \begin{aligned} \mathbf{u}^T C\mathbf{u} &= 2\hat{u} \sum_{m=1}^{\infty} \left(\sum_{\ell=1}^m \alpha_{m,\ell} \mathbf{1}^T C\mathbf{p}_\ell \right) \varepsilon^m \\ &\quad + \sum_{m=2}^{\infty} \left(\sum_{k=1}^{m-1} \sum_{\ell=1}^k \sum_{j=1}^{m-k} \alpha_{k,\ell} \alpha_{m-k,j} \mathbf{p}_\ell^T C\mathbf{p}_j \right) \varepsilon^m \end{aligned}$$

$$(2.8) \quad \mathbf{1}^T C\mathbf{u} = \sum_{m=1}^{\infty} \left(\sum_{\ell=1}^m \alpha_{m,\ell} \mathbf{1}^T C\mathbf{p}_\ell \right) \varepsilon^m.$$

Let

$$W(\varepsilon) := \varepsilon^{-1} (\mathbf{u}^T C \mathbf{u} - 2\hat{\mathbf{u}} \mathbf{1}^T C \mathbf{u}).$$

Then a necessary condition for order p is that $W(\varepsilon) = O(\varepsilon^{p+1})$ (recall that both the numerator and the denominator are $O(\varepsilon)$). Clearly, this is also sufficient if the $O(\varepsilon)$ terms therein are nonzero. Comparing (2.7) and (2.8), we have

$$(2.9) \quad \begin{aligned} W(\varepsilon) &= \sum_{m=1}^{\infty} \left(\sum_{k=1}^m \sum_{\ell=1}^k \sum_{j=1}^{m+1-k} \alpha_{k,\ell} \alpha_{m+1-k,j} \mathbf{p}_\ell^T C \mathbf{p}_j \right) \varepsilon^m \\ &= \sum_{m=1}^{\infty} \sum_{\ell=1}^m \sum_{j=1}^{m+1-\ell} \left(\sum_{k=\ell}^{m+1-j} \alpha_{k,\ell} \alpha_{m+1-k,j} \right) \mathbf{p}_\ell^T C \mathbf{p}_j \varepsilon^m. \end{aligned}$$

Moreover,

$$V(\varepsilon) = \frac{\hat{\mathbf{u}} \left[\alpha_{1,1} \mathbf{1}^T C \mathbf{p}_1 + \sum_{m=1}^{\infty} \left(\sum_{\ell=1}^{m+1} \alpha_{m+1,\ell} \mathbf{1}^T C \mathbf{p}_\ell \right) \varepsilon^m \right] + \frac{1}{2} W(\varepsilon)}{\alpha_{1,1} \mathbf{1}^T C \mathbf{p}_1 + \sum_{m=1}^{\infty} \left(\sum_{\ell=1}^{m+1} \alpha_{m+1,\ell} \mathbf{1}^T C \mathbf{p}_\ell \right) \varepsilon^m},$$

hence the method is of order at least p if $\mathbf{1}^T C \mathbf{p}_1 \neq 0$. Thus, the order is degraded for all β_1 if $C \mathbf{1} = \mathbf{0}$ and it might be degraded for particular values of β_1 if C is singular and \mathbf{p}_1 is an eigenvector corresponding to the eigenvalue 0. We impose in the sequel the requirement that $C \mathbf{1} \neq \mathbf{0}$ (i.e. that C is *nondegenerate*), W.L.O.G..

As we have already seen, $p \geq 1$ only if

$$\alpha_{1,1}^2 \mathbf{p}_1^T C \mathbf{p}_1 = 0.$$

Consequently, we require $\mathbf{q}^T C \mathbf{q} \equiv 0 \ \forall q \in \mathbb{R}$. The necessary condition for $p \geq 2$ is

$$2\alpha_{1,1} (\alpha_{2,1} \mathbf{p}_1^T C \mathbf{p}_1 + \alpha_{2,2} \mathbf{p}_1^T C \mathbf{p}_2) = 0,$$

hence we deduce that

$$(2.10) \quad \mathbf{q}_1^T C \mathbf{q}_1 \equiv \mathbf{q}_1^T C \mathbf{q}_2 \equiv 0,$$

where

$$\mathbf{q}_j = [1, q^j, q^{2j}, \dots, q^{nj}]^T, \quad j \in \mathbb{Z}^+, \quad q \in \mathbb{R}.$$

3. The General Case. We consider next $p \geq 3$. The conditions (2.10) are still necessary and the third-order terms are

$$\begin{aligned} &(2\alpha_{1,1}\alpha_{3,1} + \alpha_{2,1}^2) \mathbf{p}_1^T C \mathbf{p}_1 \\ &+ 2(\alpha_{1,1}\alpha_{3,2} + \alpha_{2,1}\alpha_{2,2}) \mathbf{p}_1^T C \mathbf{p}_2 \\ &+ 2\alpha_{1,1}\alpha_{3,3} \mathbf{p}_1^T C \mathbf{p}_3 + \alpha_{2,2}^2 \mathbf{p}_2^T C \mathbf{p}_2, \end{aligned}$$

since (2.10) implies $\mathbf{q}_2^T C \mathbf{q}_2 = 0$ (note that $\mathbf{q}_2(q) = \mathbf{q}_1(q^2)$). Hence we require just one more equation,

$$(3.1) \quad \mathbf{q}_1^T C \mathbf{q}_3 = 0.$$

Generally, by the similar reasoning, we need

$$(3.2) \quad \mathbf{q}_1^T C \mathbf{q}_i = 0, \quad i = 1, 2, \dots, p,$$

for order p . We know that the matrix C cannot be $p \times p$, it has to be larger. In the following proposition we will prove that for $N = p(p+3)/2$, the smallest matrix C satisfying (3.2) is $(N+1) \times (N+1)$. A lemma is required first.

LEMMA 3.1. *Let C be a symmetric matrix, and*

$$C = [a_{k,\ell}]_{k,\ell=0,1,\dots,K}, \quad a(t, s) = \sum_{k=0}^K \sum_{\ell=0}^K a_{k,\ell} t^k s^\ell.$$

If $a(q^j, q^i) = 0$, $1 \leq i \leq j$, i and j are relatively prime, then $(t^i - s^j) | a(t, s)$.

Proof. Let us consider the coefficients $a_{k,\ell}$ of $a(t, s)$. Since

$$\begin{aligned} 0 &= a(q^j, q^i) = \sum_{k=0}^K \sum_{\ell=0}^K a_{k,\ell} q^{jk} q^{i\ell} \\ &= \sum (a_{k,\ell} + a_{k-i,\ell+j} + a_{k-2i,\ell+2j} + \dots + a_{k-ui,\ell+uj}) q^{jk+i\ell}, \end{aligned}$$

every coefficient of $q^{jk+i\ell}$ has to be zero for $0 \leq k \leq K$, $0 \leq \ell \leq K$. That means, using the fact that $\gcd(i, j) = 1$ (hence each coefficient appears only in one equation) that

$$a_{k,\ell} + a_{k-i,\ell+j} + a_{k-2i,\ell+2j} + \dots + a_{k-ui,\ell+uj} = 0,$$

where all subscripts are bounded by 0 and K . Notice that there are complex numbers $a_1, a_2, \dots, a_u, b_1, b_2, \dots, b_u$ such that

$$\begin{aligned} &a_{k,\ell} t^k s^\ell + a_{k-i,\ell+j} t^{k-i} s^{\ell+j} + a_{k-2i,\ell+2j} t^{k-2i} s^{\ell+2j} + \dots + a_{k-ui,\ell+uj} t^{k-ui} s^{\ell+uj} \\ &= t^{k-ui} s^{\ell+uj} (a_1 t^i s^{-j} + b_1) (a_2 t^i s^{-j} + b_2) \dots (a_u t^i s^{-j} + b_u) \\ &= t^{k-ui} s^\ell (a_1 t^i + b_1 s^j) (a_2 t^i + b_2 s^j) \dots (a_u t^i + b_u s^j). \end{aligned}$$

Substituting $t = 1$ and $s = 1$ we get

$$0 = a_{k,\ell} + a_{k-i,\ell+j} + a_{k-2i,\ell+2j} + \dots + a_{k-ui,\ell+uj} = (a_1 + b_1)(a_2 + b_2) \dots (a_u + b_u).$$

One of $(a_m + b_m)$ s must be zero and, without loss of generality, we assume that it is the first. Hence $a_1 = -b_1$ (notice that also a_1 could be zero) and

$$\begin{aligned} &a_{k,\ell} t^k s^\ell + a_{k-i,\ell+j} t^{k-i} s^{\ell+j} + a_{k-2i,\ell+2j} t^{k-2i} s^{\ell+2j} + \dots + a_{k-ui,\ell+uj} t^{k-ui} s^{\ell+uj} \\ &= t^{k-ui} s^\ell a_1 (t^i - s^j) (a_2 t^i + b_2 s^j) \dots (a_u t^i + b_u s^j). \end{aligned}$$

Let u, v be integers such that $0 \leq K - vi < i$ and $0 \leq K - uj < j$, respectively. We deduce that (the second sum being unique, because of $\gcd(i, j) = 1$)

$$\begin{aligned} a(t, s) &= \sum_{k=0}^K \sum_{\ell=0}^K a_{k,\ell} t^k s^\ell \\ &= \sum_{k_1=0}^{i-1} \sum_{\ell_1=0}^{j-1} \left[\sum_{k_2=0}^v (a_{k_1+k_2i, \ell_1} t^{k_1+k_2i} s^{\ell_1} + a_{k_1+(k_2-1)i, \ell_1+j} t^{k_1+(k_2-1)i} s^{\ell_1+j} \right. \end{aligned}$$

$$\begin{aligned}
& + a_{k_1+(k_2-2)i, \ell_1+2j} t^{k_1+(k_2-2)i} s^{\ell_1+2j} + \dots \\
& + a_{k_1+(k_2-k_2)i, \ell_1+k_2j} t^{k_1+(k_2-k_2)i} s^{\ell_1+k_2j} \\
& + \sum_{\ell_2=1}^u (a_{k_1+v_i, \ell_1+\ell_2j} t^{k_1+v_i} s^{\ell_1+\ell_2j} + a_{k_1+(v-1)i, \ell_1+(\ell_2+1)j} t^{k_1+(v-1)i} s^{\ell_1+(\ell_2+1)j} \\
& + a_{k_1+(v-2)i, \ell_1+(\ell_2+2)j} t^{k_1+(v-2)i} s^{\ell_1+(\ell_2+2)j} + \dots \\
& + a_{k_1+(v-u+\ell_2)i, \ell_1+u_j} t^{k_1+(v-u+\ell_2)i} s^{\ell_1+u_j}] \\
& = (t^i - s^j) \sum b_{k, \ell} t^k s^\ell
\end{aligned}$$

where if a subscript of $a_{k, \ell}$ is $> K$, then the $a_{k, \ell}$ in question is defined to be zero. \square

PROPOSITION 3.2. *Let $N_p := p(p+3)/2$. The smallest C satisfying the system of equations*

$$(3.3) \quad \mathbf{q}_1^T C \mathbf{q}_i = 0, \quad i = 1, 2, \dots, p, \quad \text{where } \mathbf{q}_i = [1, q^i, q^{2i}, \dots, q^{ni}]^T, \quad i \in \mathbb{Z}^+, \quad q \in \mathbb{R}$$

is $(N_p + 1) \times (N_p + 1)$. Furthermore, let C_{N_p} be the smallest C corresponding to p , then we can construct C_{N_p} from $C_{N_{p-1}}$ according to the following prescription.

$$\begin{aligned}
(3.4) \quad C_{N_1} &= \begin{bmatrix} 0 & 0 & 1 \\ 0 & -2 & 0 \\ 1 & 0 & 0 \end{bmatrix}, \\
C_{N_p} &= \begin{bmatrix} O_{(p+1) \times N_{p-1}} & O_{(p+1) \times (p+1)} \\ C_{N_{p-1}} & O_{N_{p-1} \times (p+1)} \end{bmatrix} + \begin{bmatrix} C_{N_{p-1}} & O_{N_{p-1} \times (p+1)} \\ O_{(p+1) \times N_{p-1}} & O_{(p+1) \times (p+1)} \end{bmatrix} \\
&\quad - \begin{bmatrix} O_{1 \times 1} & O_{1 \times N_{p-1}} & O_{1 \times p} \\ O_{N_{p-1} \times 1} & C_{N_{p-1}} & O_{N_{p-1} \times p} \\ O_{p \times 1} & O_{p \times N_{p-1}} & O_{p \times p} \end{bmatrix} - \begin{bmatrix} O_{p \times p} & O_{p \times N_{p-1}} & O_{p \times 1} \\ O_{N_{p-1} \times p} & C_{N_{p-1}} & O_{N_{p-1} \times 1} \\ O_{1 \times p} & O_{1 \times N_{p-1}} & O_{1 \times 1} \end{bmatrix},
\end{aligned}$$

where $p \geq 2$ and $O_{i \times j}$ is a zero matrix of order $i \times j$. Furthermore,

$$(3.5) \quad v_p(q) := \mathbf{1}^T C_{N_p} \mathbf{q}_1 = (1-q)^p \prod_{k=1}^p (1-q^k).$$

Proof. We proceed by induction. By direct calculation, $\mathbf{q}_1^T C_{N_1} \mathbf{q}_1 = 0$. Assume next that $\mathbf{q}_1^T C_{N_{p-1}} \mathbf{q}_i = 0$ for $i = 1, 2, \dots, p-1$. Then

$$\begin{aligned}
\mathbf{q}_1^T C_{N_p} \mathbf{q}_i &= q^{p+1} \mathbf{q}_1^T C_{N_{p-1}} \mathbf{q}_i + \mathbf{q}_1^T C_{N_{p-1}} q^{i(p+1)} \mathbf{q}_i - q^1 \mathbf{q}_1^T C_{N_{p-1}} q^i \mathbf{q}_i \\
&\quad - q^p \mathbf{q}_1^T C_{N_{p-1}} q^{i \cdot p} \mathbf{q}_i = 0,
\end{aligned}$$

for $i = 1, 2, \dots, p-1$. Furthermore,

$$\begin{aligned}
\mathbf{q}_1^T C_{N_p} \mathbf{q}_p &= q^{p+1} \mathbf{q}_1^T C_{N_{p-1}} \mathbf{q}_p + \mathbf{q}_1^T C_{N_{p-1}} q^{p(p+1)} \mathbf{q}_p - q^1 \mathbf{q}_1^T C_{N_{p-1}} q^p \mathbf{q}_p \\
&\quad - q^p \mathbf{q}_1^T C_{N_{p-1}} q^{p \cdot p} \mathbf{q}_p = 0.
\end{aligned}$$

Hence $\mathbf{q}_1^T C_{N_p} \mathbf{q}_i = 0$, for $i = 1, 2, \dots, p$ and any positive integer p .

To prove that N_p is the smallest number such that there is at least one non-trivial C satisfying (3.2), we write $\mathbf{S} = [1, s, \dots, s^n]^T$ and

$$b_i(q, s) = \mathbf{q}_1^T C_{N_i} \mathbf{S}, \quad i = 1, 2, \dots, p.$$

Then by our assumption

$$b_p(q, q^i) = \mathbf{q}_1^T C_{N_p} \mathbf{q}_i = 0, \quad i = 1, 2, \dots, p.$$

Hence, by the Lemma 3.1, $(s - q^i)|b_p(q, s)$, $i = 1, 2, \dots, p$. Note that $b_p(q, s)$ is a symmetric function of q and s , thus

$$\prod_{k=1}^p [(s - q^k)(q - s^k)] | b_p(q, s).$$

On the other hand, by our recursion,

$$\begin{aligned} b_1(q, s) &= \mathbf{q}_1^T C_{N_1} \mathbf{S} = q^2 - 2sq + s^2 = (q - s)(q - s), \\ b_p(q, s) &= \mathbf{q}_1^T C_{N_p} \mathbf{S} \\ &= q^{p+1} \mathbf{q}_1^T C_{N_{p-1}} \mathbf{S} + \mathbf{q}_1^T C_{N_{p-1}} s^{p+1} \mathbf{S} - q \mathbf{q}_1^T C_{N_{p-1}} s \mathbf{S} - q^p \mathbf{q}_1^T C_{N_{p-1}} s^p \mathbf{S} \\ &= (q^{p+1} + s^{p+1} - qs - q^p s^p) \mathbf{q}_1^T C_{N_{p-1}} \mathbf{S} \\ &= (q^p - s)(q - s^p) b_{p-1}(q, s) \\ &= \prod_{k=1}^p [(q^k - s)(q - s^k)] \quad (\text{by induction}) \\ &= (-1)^p \prod_{k=1}^p [(s - q^k)(q - s^k)]. \end{aligned}$$

Thus $b_p(q, s)$ is the lowest degree $b(q, s)$ satisfying our assumption. The highest power of s or q in it, which corresponds to the smallest degree of matrix C , is

$$N_p = p + 1 + 2 + \dots + p = \frac{1}{2}p(p + 3).$$

The next statement is obvious,

$$v_p(q) = b_p(q, 1) = \prod_{k=1}^p [(q^k - 1)(q - 1)] = (1 - q)^p \prod_{k=1}^p (1 - q^k).$$

The proof is complete. \square

To ensure that

$$W(\varepsilon) := \varepsilon^{-1} (\mathbf{u}^T C \mathbf{u} - 2\hat{\mathbf{u}} \mathbf{1}^T C \mathbf{u}) = O(\varepsilon^{p+1}),$$

it is necessary that (3.3) holds. However, for $p = 4$, (3.3) is not sufficient and we need one more equation,

$$(3.6) \quad \mathbf{q}_2^T C \mathbf{q}_3 = 0.$$

Generally, to guarantee $p \geq 4$,

$$(3.7) \quad \mathbf{q}_i^T C \mathbf{q}_j = 0, \quad 2 \leq i + j \leq p + 1, \quad 1 \leq i, j \leq p.$$

have to hold too. Thus, when p gets larger, our matrix C gets quite large. Fortunately, it is still possible to construct C recursively.

THEOREM 3.3. *Let*

$$\mathbf{J}_p := \{k : 1 \leq k \leq \lfloor p/2 \rfloor; k \text{ and } p+1-k \text{ are relatively prime}\} =: \{k_1, k_2, \dots, k_{J_p}\}$$

where $k_1 = 1$ and J_p is the number of elements in \mathbf{J}_p . Let

$$M_1 = 2,$$

$$M_p = M_{p-1} + J_p(p+1) = \sum_{k=1}^{\lfloor p/2 \rfloor} \sum_{\ell=k, \gcd(\ell,k)=1}^{p+1-k} (\ell+k), \quad p \geq 2,$$

$$a_1(t, s) = (t-s)^2,$$

$$\begin{aligned} a_p(t, s) &= a_{p-1}(t, s) \prod_{j=1}^{J_p} (t^{k_j} - s^{p+1-k_j})(t^{p+1-k_j} - s^{k_j}) \\ &= \prod_{k=1}^{\lfloor p/2 \rfloor} \prod_{\ell=k, \gcd(\ell,k)=1}^{p+1-k} (t^\ell - s^k)(t^k - s^\ell) := \sum_{i=0}^{M_p} \sum_{j=0}^{M_p} c_{i,j} t^i s^j \quad p \geq 2. \end{aligned}$$

Then $C = [c_{i,j}]_{i,j=0,1,\dots,M_p}$ is the smallest matrix satisfying (3.7).

We can construct C by the following recursive scheme. Let

$$C_{M_1} = \begin{bmatrix} 0 & 0 & 1 \\ 0 & -2 & 0 \\ 1 & 0 & 0 \end{bmatrix}.$$

For $p \geq 2$, let $M_{p,i} = M_{p-1} + i(p+1)$, $i = 0, 1, \dots, J_p$, $M_p := M_{p,J_p}$, and set $C_{M_p,0} := C_{M_{p-1}}$. Then for $i = 1, 2, \dots, J_p$,

$$\begin{aligned} C_{M_p,i} &= \begin{bmatrix} O_{(p+1) \times M_{p,i-1}} & O_{(p+1) \times (p+1)} \\ C_{M_{p,i-1}} & O_{M_{p,i-1} \times (p+1)} \end{bmatrix} + \begin{bmatrix} O_{M_{p,i-1} \times (p+1)} & C_{M_{p,i-1}} \\ O_{(p+1) \times (p+1)} & O_{(p+1) \times M_{p,i-1}} \end{bmatrix} \\ &- \begin{bmatrix} O_{k_i \times k_i} & O_{k_i \times M_{p,i-1}} & O_{k_i \times (p+1-k_i)} \\ O_{M_{p,i-1} \times k_i} & C_{M_{p,i-1}} & O_{M_{p,i-1} \times (p+1-k_i)} \\ O_{(p+1-k_i) \times k_i} & O_{(p+1-k_i) \times M_{p,i-1}} & O_{(p+1-k_i) \times (p+1-k_i)} \end{bmatrix} \\ &- \begin{bmatrix} O_{(p+1-k_i) \times (p+1-k_i)} & O_{(p+1-k_i) \times M_{p,i-1}} & O_{(p+1-k_i) \times k_i} \\ O_{M_{p,i-1} \times (p+1-k_i)} & C_{M_{p,i-1}} & O_{M_{p,i-1} \times k_i} \\ O_{k_i \times (p+1-k_i)} & O_{k_i \times M_{p,i-1}} & O_{k_i \times k_i} \end{bmatrix}. \end{aligned}$$

Furthermore,

$$v_p(q) = v_{p-1}(q) \prod_{i=1}^{J_p} (1 - q^{k_i})(1 - q^{p+1-k_i}) = \prod_{k=1}^{\lfloor p/2 \rfloor} \prod_{\ell=k, \gcd(\ell,k)=1}^{p+1-k} (1 - q^\ell)(1 - q^k).$$

Proof. The proof is straightforward. Suppose $1 \leq i \leq p$, $1 \leq j \leq p$, $2 \leq i+j \leq p+1$. If $\gcd(i, j) = 1$, then the factor $(t^i - s^j)$ is a divisor of $a_p(t, s)$, thus

$$\mathbf{q}_i^T C \mathbf{q}_j = a_p(q^j, q^i) = 0.$$

On the other hand, if $\gcd(i, j) = \sigma \geq 2$ then $i = k\sigma$, $j = l\sigma$ and $1 \leq k, l < p$, $2 \leq k + l < p + 1$, and we still have

$$\mathbf{q}_i^T C \mathbf{q}_j = \mathbf{q}_k^T C \mathbf{q}_l = a_p(q^l, q^k) = 0.$$

Hence (3.7) is satisfied.

Furthermore, our Lemma 3.1 guarantees that $C = C_{M_p}$ is the smallest matrix satisfying (3.7).

We can get our recursive scheme for C from the recurrence formula for $a_p(t, s)$. The last statement is obvious considering $v_p(t) = a_p(1, t)$. \square

As for $n \geq M_p + 1$, we can find more than one matrix C that satisfies (3.7).

PROPOSITION 3.4. *Let \mathcal{C}_p^n be the space of matrices satisfying (3.7). The dimension of \mathcal{C}_p^n is $(n - M_p + 1)(n - M_p + 2)/2$, where M_p has been defined in Theorem 3.3. Furthermore, for fixed p and M_p , we can construct a base of \mathcal{C}_p^n in the following way. There is one element, up to a constant multiple, in $\mathcal{C}_p^{M_p}$ as constructed before, which we write as C_{M_p} . All the three elements in $\mathcal{C}_p^{M_p+1}$ can be written in the form*

$$\begin{aligned} C_{M_p+1}^{(1)} &= \begin{bmatrix} O_{1 \times M_p+1} & 0 \\ C_{M_p} & O_{M_p+1 \times 1} \end{bmatrix} + \begin{bmatrix} O_{M_p+1 \times 1} & C_{M_p} \\ 0 & O_{1 \times M_p+1} \end{bmatrix}, \\ C_{M_p+1}^{(2)} &= \begin{bmatrix} 0 & O_{1 \times M_p+1} \\ O_{M_p+1 \times 1} & C_{M_p} \end{bmatrix}, \quad C_{M_p+1}^{(3)} = \begin{bmatrix} C_{M_p} & O_{M_p+1 \times 1} \\ O_{1 \times M_p+1} & 0 \end{bmatrix}. \end{aligned}$$

Furthermore,

$$\begin{aligned} v_{p,p+1}^{(0)}(q) &= \mathbf{1}^T C_{M_p+1}^{(1)} \mathbf{q}_1 = \mathbf{1}^T C_{M_p} \mathbf{q}_1 + \mathbf{1}^T C_{M_p} q \mathbf{q}_1 = (1 + q)v_p(q); \\ v_{p,p+1}^{(1)}(q) &= \mathbf{1}^T C_{M_p+1}^{(2)} \mathbf{q}_1 = \mathbf{1}^T C_{M_p} q \mathbf{q}_1 = qv_p(q); \\ v_{p,p+1}^{(2)}(q) &= \mathbf{1}^T C_{M_p+1}^{(3)} \mathbf{q}_1 = \mathbf{1}^T C_{M_p} \mathbf{q}_1 = v_p(q). \end{aligned}$$

For general $n \geq M_p + 1$ we can construct a base of \mathcal{C}_p^n by recursion. Let $L = n - M_p$. First we construct one matrix of $(M_p + k + 1) \times (M_p + k + 1)$ by enlarging C_{M_p} in the following fashion,

$$\begin{aligned} C_{M_p,0}^{(0)} &= C_{M_p}; \\ C_{M_p+k,k}^{(0)} &= \begin{bmatrix} O_{1 \times M_p+k} & 0 \\ C_{M_p+k-1,k-1}^{(0)} & O_{M_p+k \times 1} \end{bmatrix} + \begin{bmatrix} O_{M_p+k \times 1} & C_{M_p+k-1,k-1}^{(0)} \\ 0 & O_{1 \times M_p+k} \end{bmatrix} \end{aligned}$$

for $k = 1, 2, \dots, L$. We augment each to a matrix of size $(M_p + L + 1) \times (M_p + L + 1)$ by adding $L - k$ zero rows and columns as follows, whereby they are all linearly independent.

$$\begin{aligned} C_{M_p+L,k}^{(i)} &= \begin{bmatrix} O_{i \times i} & O_{i \times M_p+k+1} & O_{i \times L-k-i} \\ O_{M_p+k+1 \times i} & C_{M_p+k,k}^{(0)} & O_{M_p+k+1 \times L-k-i} \\ O_{L-k-i \times i} & O_{L-k-i \times M_p+k+1} & O_{L-k-i \times L-k-i} \end{bmatrix}, \\ & i = 0, 1, \dots, L - k, \quad k = 0, 1, 2, \dots, L. \end{aligned}$$

Correspondingly, $v_{p,n}^{(i,k)}(q) := \mathbf{1}^T C_{M_p+L,k}^{(i)} \mathbf{q}_1 = q^i (1 + q)^k v_p(q)$, $i = 0, 1, 2, \dots, L - k$, $k = 0, 1, 2, \dots, L$.

Proof. Let $C \in \mathcal{C}_p^n$ and

$$b(q, s) = \mathbf{q}_1^T C \mathbf{S}.$$

Then, according to the lemma,

$$\prod_{k=1}^{[p/2]} \prod_{\ell=k, \gcd(\ell, k)=1}^{p+1-k} (q^\ell - s^k)(q^k - s^\ell) |b(q, s).$$

Hence

$$b(q, s) = \prod_{k=1}^{[p/2]} \prod_{\ell=k, \gcd(\ell, k)=1}^{p+1-k} (q^\ell - s^k)(q^k - s^\ell) r(q, s),$$

where $r(s, q)$ is a polynomial of degree $n - M_p$ in two variables. There are $(n - M_p + 1)(n - M_p + 2)/2$ unknowns for $r(t, s)$, that is the upper bound for the dimension of \mathcal{C}_p^n . It is obvious that our construction gives $(n - M_p + 1)(n - M_p + 2)/2$ linearly independent matrices. Thus our assertions are true. \square

THEOREM 3.5. *If we choose $C \in \mathcal{C}_p^{M_p}$ as in Theorem 3.3 or $C \in \mathcal{C}_p^n$ as in Proposition 3.4, then the quadratic model*

$$G(z) = \frac{\mathbf{u}^T C \mathbf{u}}{2\mathbf{1}^T C \mathbf{u}}$$

has at least order p , unless β_1 is a root of unity.

Examples. For $p = 2$, $n = 5$, C is

$$(3.8) \quad \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & -1 & -2 & 0 \\ 0 & 0 & 2 & 1 & -1 & 0 \\ 0 & -1 & 1 & 2 & 0 & 0 \\ 0 & -2 & -1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}.$$

For $p = 2$, $n = 6$, all the C s are

$$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & -1 & -2 & 0 \\ 0 & 0 & 0 & 2 & 1 & -1 & 0 \\ 0 & 0 & -1 & 1 & 2 & 0 & 0 \\ 0 & 0 & -2 & -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}; \quad \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 & -2 & 0 & 0 & 0 \\ 0 & 0 & 2 & 1 & -1 & 0 & 0 & 0 \\ 0 & -1 & 1 & 2 & 0 & 0 & 0 & 0 \\ 0 & -2 & -1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}; \quad \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & -1 & -1 & 0 & 0 \\ 0 & 0 & 0 & 1 & -1 & -1 & 0 & 0 \\ 0 & 0 & 1 & 2 & 1 & 0 & 0 & 0 \\ 0 & -1 & -1 & 1 & 0 & 0 & 0 & 0 \\ 0 & -1 & -1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}.$$

For $p = 2$, $n = 7$, the C s are

$$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & -1 & -2 & 0 & 0 \\ 0 & 0 & 0 & 2 & 1 & -1 & 0 & 0 \\ 0 & 0 & -1 & 1 & 2 & 0 & 0 & 0 \\ 0 & 0 & -2 & -1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}; \quad \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 & -2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 1 & -1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 1 & 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & -2 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}; \quad \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & -1 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & -1 & -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 2 & 1 & 0 & 0 & 0 & 0 \\ 0 & -1 & -1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix};$$

$$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & -1 & -2 & 0 \\ 0 & 0 & 0 & 2 & 1 & -1 & 0 \\ 0 & 0 & -1 & 1 & 2 & 0 & 0 \\ 0 & 0 & -2 & -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \end{bmatrix}; \quad \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & -1 & -1 & 0 \\ 0 & 0 & 0 & 0 & 1 & -1 & -1 \\ 0 & 0 & 0 & 1 & 2 & 1 & 0 \\ 0 & 0 & -1 & -1 & 1 & 0 & 0 \\ 0 & 0 & -1 & -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}; \quad \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -2 & -1 & 0 \\ 0 & 0 & 0 & 2 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 2 & 0 & 0 \\ 0 & -1 & -2 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}.$$

Finally, for $p = 3$, $n = 9$, the matrix C is

$$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & -1 & -2 \\ 0 & 0 & 0 & 0 & 1 & 2 & 2 & 1 & -1 \\ 0 & 0 & 0 & -2 & -1 & 0 & 1 & 2 & -1 \\ 0 & 0 & 1 & -1 & -2 & -1 & 0 & 2 & 0 \\ 0 & 0 & 2 & 0 & -1 & -2 & -1 & 1 & 0 \\ 0 & -1 & 2 & 1 & 0 & -1 & -2 & 0 & 0 \\ 0 & -1 & 1 & 2 & 2 & 1 & 0 & 0 & 0 \\ 0 & -2 & -1 & -1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}.$$

Let us study next the attractivity of $G_N(z)$.

THEOREM 3.6. *Given $p > 0$. Let*

$$\begin{aligned} \mathbf{J}_p &:= \{k : 1 \leq k \leq [p/2]; k \text{ and } p+1-k \text{ are relatively prime}\} = \{k_1, k_2, \dots, k_{J_p}\}, \\ S_p &= k_1 + \dots + k_{J_p}, \\ K_p &= S_1 + \dots + S_p, \end{aligned}$$

where $k_1 = 1$ and J_p is the number of elements in \mathbf{J}_p . If $f(z)$ is super-attractive of degree $s \geq 1$ at the fixed point \hat{z} , then $G_{M_p}(z)$ is super-attractive there of the degree $2(s+1)^{K_p} - 2$.

Proof. Without loss of generality we suppose that $\hat{z} = 0$. If

$$f(z) = \alpha_0 z^{s+1} + O(z^{s+2}),$$

then by induction we have

$$f^{\circ m}(z) = \alpha_m z^{(s+1)^m} + O(z^{(s+1)^m+1}).$$

Note that

$$G_{M_p}(z) = \frac{\mathbf{u}^T C_{M_p} \mathbf{u}}{2\mathbf{1}^T C_{M_p} \mathbf{u}} = \frac{\sum_{i,j} c_{i,j} f^{\circ i} f^{\circ j}}{2 \sum_{i,j} c_{i,j} f^{\circ i}}.$$

By the construction of C_{M_p} we can see that $c_{i,j} = 0$ for $0 \leq i+j \leq 2(K_p) - 1$ and $c_{K_p, K_p} \neq 0$. Among the terms of $c_{i,j} f^{\circ i} f^{\circ j}$ the smallest power of z is in the form $c_{i,j} z^{(s+1)^i + (s+1)^j}$ when $s \geq 1$, for $2K_p \leq i+j \leq 2M_p$. Furthermore, $\sum_{j=0}^{M_p} c_{0,j} = c_{0, M_p} = 1$. Thus,

$$\begin{aligned} G_{M_p}(z) &= \frac{c_{K_p, K_p} \alpha_{K_p}^2 z^{2(s+1)^{K_p}} + O(z^{2(s+1)^{K_p}+1})}{c_{0, M_p} z + O(z^2)} \\ &= c_{K_p, K_p} \alpha_{K_p}^2 z^{2(s+1)^{K_p}-1} + O(z^{2(s+1)^{K_p}}). \quad \square \end{aligned}$$

COROLLARY. *Let*

$$G_{n,p}(z) = \frac{\mathbf{u}^T C_{n,0}^{(n-M_p)} \mathbf{u}}{2\mathbf{1}^T C_{n,0}^{(n-M_p)} \mathbf{u}}$$

with $C_{n,0}^{(n-M_p)}$ as in Proposition 3.4, then if $f(z)$ is super-attractive of degree $s \geq 1$ at the fixed point \hat{z} then $G_{n,p}(z)$ is super-attractive there of degree $2(s+1)^{n-M_p+K_p} - (s+1)^{n-M_p} - 1$.

4. The fixed point at ∞ . Let f be analytic for $|z| \geq 1$ and $\infty \in F_f$. Assume that

$$f(z) = \gamma_0 z + \sum_{k=1}^{\infty} \frac{1}{k!} \gamma_k z^{-k+1}.$$

For the time being, we assume that γ_0 is neither zero nor a root of unity. Then the Taylor expansion of $f^{\circ m}$ about ∞ is

$$f^{\circ m}(z) = \gamma_0^m z + \sum_{k=1}^{\infty} \frac{1}{k!} \epsilon_k^{(m)} z^{-k+1} \quad m = 1, 2, \dots$$

According to Iserles [2], there exist numbers $D_{k,l}$, $l = 0, 1, \dots, k$, $k = 0, 1, \dots$, dependent on $\{\gamma_k\}_{k=1}^{\infty}$ but not on m , such that

$$\epsilon_k^{(m+1)} = \sum_{l=0}^k D_{k,l} \epsilon_l^{(m)}.$$

Moreover, $D_{k,k} = \gamma_0^{1-k}$, $k = 0, 1, \dots$. Let

$$\begin{aligned} B_{1,1} &= 1, \\ B_{k,l} &= \frac{1}{\gamma_0^l - \gamma_0^{1-k}} \sum_{j=1-l}^{k-1} D_{k,j} B_{j,l}, \quad l = 2-k, 3-k, \dots, 1, \quad k = 1, 2, \dots, \\ B_{k,1-k} &= \gamma_0^{k-1} \left(\gamma_k - \sum_{l=2-k}^1 B_{k,l} \gamma_0^l \right), \quad k = 1, 2, \dots \end{aligned}$$

Then

$$\epsilon_k^{(m)} = \sum_{l=1-k}^1 B_{k,l} \gamma_0^{lm} \quad k, m = 0, 1, \dots$$

Therefore if $\mathbf{p}_1^T C \mathbf{p}_1 = 0$, $\mathbf{1}^T C \mathbf{p}_1 \neq 0$, then

$$G(z) = \frac{\mathbf{u}^T C \mathbf{u}}{2\mathbf{1}^T C \mathbf{u}} = \frac{\mathbf{p}_1^T C \mathbf{p}_1 z^2 + 2B_{1,0} \mathbf{1}^T C \mathbf{p}_1 z + O(1)}{2\mathbf{1}^T C \mathbf{p}_1 z + \sum_{k=1}^{\infty} \frac{1}{k!} \sum_{l=1-k}^1 B_{k,l} \mathbf{1}^T C \mathbf{p}_1 z^{-k+1}} = B_{1,0} + O(z^{-1}).$$

In the case when ∞ is a super-attractive fixed point of f of degree s , we write

$$f(z) = \gamma_0 z^s + O(z^{s-1}).$$

Then

$$f^{\circ m}(z) = \gamma_0^{(m)} z^{s^m} + O(z^{s^m-1}).$$

Note the highest power among $z^{s^i+s^j}$, for $1 \leq i, j \leq M_p$, must be located at $i = M_p$ or $j = M_p$ and the fact that in the matrix C_{M_p} , $c_{M_p,i} = c_{i,M_p} = 0$ for $1 \leq i \leq M_p$. Therefore we get

$$\begin{aligned} G_{M_p}(z) &= \frac{\mathbf{u}^T C_{M_p} \mathbf{u}}{2\mathbf{1}^T C_{M_p} \mathbf{u}} = \frac{\sum_{i,j} c_{i,j} f^{\circ i}(z) f^{\circ j}(z)}{2 \sum_{i,j} c_{i,j} f^{\circ i}(z)} \\ &= \frac{2c_{0,M_p} \gamma_0^{(M_p)} z^{s^{M_p}+1} + O(z^{s^{M_p}})}{2c_{0,M_p} \gamma_0^{(M_p)} z^{s^{M_p}} + O(z^{s^{M_p}-1})} = z + O(1). \end{aligned}$$

We have thus deduced the following result.

PROPOSITION 4.1. *If ∞ is a fixed point of f which is neither neutral with γ_0 a root of unity nor super-attractive, then ∞ is not a fixed point of $G_{M_p}(z)$ for*

$$G_{M_p}(z) = \frac{\mathbf{u}^T C_{M_p} \mathbf{u}}{2\mathbf{1}^T C_{M_p} \mathbf{u}}$$

PROPOSITION 4.2. *If ∞ is a super-attractive fixed point of f with $s \geq 2$, then ∞ is a fixed point with degree 1 of $G_{M_p}(z)$ for*

$$G_{M_p}(z) = \frac{\mathbf{u}^T C_{M_p} \mathbf{u}}{2\mathbf{1}^T C_{M_p} \mathbf{u}}$$

For a general $n \geq M_p + 1$, we choose $C_{n,0}^{(n-M_p)} \in \mathcal{C}_p^n$ and $p \geq 1$, since

$$\begin{aligned} G_{n,p}(z) &= \frac{\mathbf{u}^T C_{n,0}^{(n-M_p)} \mathbf{u}}{2\mathbf{1}^T C_{n,0}^{(n-M_p)} \mathbf{u}} = \frac{\sum_{i,j} c_{i,j} f^{\circ i}(z) f^{\circ j}(z)}{2 \sum_{i,j} c_{i,j} f^{\circ i}(z)} \\ &= \frac{2c_{n-M_p,n} \gamma_0^{(n-M_p)} \gamma_0^{(n)} z^{s^{n-M_p}+s^n} + O(z^{s^{n-M_p}+s^n-1})}{2c_{n-M_p,n} \gamma_0^{(n)} z^{s^n} + O(z^{s^n-1})} \\ &= \gamma_0^{(n-M_p)} z^{s^{n-M_p}} + O(z^{s^{n-M_p}-1}), \end{aligned}$$

the point ∞ is still a super-attractive fixed point up to degree $s^{n-M_p} - 1$.

PROPOSITION 4.3. *If ∞ is a fixed point of f which is neither neutral with γ_0 a root of unity nor super-attractive, then ∞ is not a fixed point of $G(z)$ for*

$$G(z) = \frac{\mathbf{u}^T C \mathbf{u}}{2\mathbf{1}^T C \mathbf{u}} \quad \text{where } C \in \mathcal{C}_p^n \quad \text{and } p \geq 1; \quad n \geq M_p + 1.$$

If ∞ is a super-attractive fixed point of f with degree $s \geq 2$ then ∞ is a super-attractive fixed point of degree up to $s^{n-M_p} - 1$ for the same $G(z)$ as above.

5. The behaviour for $\beta_1 = 1$. Supposing that

$$f(z) = z + \sum_{\ell=2}^{\infty} \frac{1}{\ell!} \beta_{\ell} z^{\ell}$$

where, again, f^{om} is the m th iterant of f , it follows from [1] that there exist constants $r_{\ell,j}$ such that

$$(5.1) \quad f^{om}(z) = z + \sum_{\ell=2}^{\infty} \left(\sum_{j=1}^{\ell-1} r_{\ell,j} m^j \right) z^{\ell}, \quad m \in \mathbb{Z}^+,$$

where

$$r_{\ell,\ell-1} = \left(\frac{\beta_2}{2} \right)^{\ell-1}, \quad \ell = 2, 3, \dots$$

Suppose that $C \in \mathcal{C}_1^n$. Differentiating $\mathbf{q}_1^T C \mathbf{q}_1 \equiv 0$ with respect to q we obtain

$$\mathbf{q}_1^T C \mathbf{q}'_1 \equiv 0,$$

hence, letting $q = 1$,

$$(5.2) \quad \mathbf{1}^T C \mathbf{k}_1 = 0,$$

where

$$\mathbf{k}_{\ell}^T := [0^{\ell} \ 1^{\ell} \ 2^{\ell} \ \dots \ n^{\ell}], \quad \ell \in \mathbb{Z}^+.$$

Differentiating again, we have

$$\mathbf{q}_1^T C \mathbf{q}_1'' + \mathbf{q}'_1{}^T C \mathbf{q}'_1 = 0,$$

hence, because of (5.2),

$$(5.3) \quad \mathbf{1}^T C \mathbf{k}_2 + \mathbf{k}_1^T C \mathbf{k}_1 = 0.$$

Because of (5.1), we have

$$\mathbf{u} = \mathbf{1}z + \sum_{\ell=2}^{\infty} \left(\sum_{j=1}^{\ell-1} r_{\ell,j} \mathbf{k}_j \right) z^{\ell}.$$

Thus, taking (5.2) into account,

$$\begin{aligned} \mathbf{1}^T C \mathbf{u} &= \sum_{\ell=3}^{\infty} \left(\sum_{j=2}^{\ell-1} r_{\ell,j} \mathbf{1}^T C \mathbf{k}_j \right) z^{\ell}, \\ \mathbf{u}^T C \mathbf{u} &= 2 \sum_{\ell=3}^{\infty} \left(\sum_{j=2}^{\ell-1} r_{\ell,j} \mathbf{1}^T C \mathbf{k}_j \right) z^{\ell+1} + \sum_{\ell_1=2}^{\infty} \sum_{\ell_2=2}^{\infty} \sum_{j_1=1}^{\ell_1-1} \sum_{j_2=1}^{\ell_2-1} r_{\ell_1,j_1} r_{\ell_2,j_2} \mathbf{k}_{j_1}^T C \mathbf{k}_{j_2} z^{\ell_1+\ell_2}. \end{aligned}$$

Recall that the function that we are iterating is

$$G_n(z) := \frac{1}{2} \frac{\mathbf{u}^T C \mathbf{u}}{\mathbf{1}^T C \mathbf{u}}.$$

In our case

$$G_n(z) = z \left(1 + \frac{r_{2,1}^2 \mathbf{k}_1^T C \mathbf{k}_1 + O(z)}{2r_{3,2} \mathbf{1}^T C \mathbf{k}_2 + O(z)} \right).$$

Thus, unless $\mathbf{k}_1^T C \mathbf{k}_1 = 0$, (5.3) yields

$$G_n(z) = \frac{1}{2}z + O(z^2).$$

In other words, the fixed point is merely attractive (not super-attractive!) and $G'_1(0) = \frac{1}{2}$. This is identical to the standard Steffensen method [2].

The remaining case is

$$(5.4) \quad \mathbf{k}_1^T C \mathbf{k}_1 = \mathbf{1}^T C \mathbf{k}_2 = 0.$$

Considering the third derivative of $\mathbf{q}_1^T C \mathbf{q}_1 \equiv 0$, we readily affirm (taking into account (5.2)–(5.4)) that

$$(5.5) \quad \mathbf{1}^T C \mathbf{k}_3 + 3\mathbf{k}_1^T C \mathbf{k}_2 = 0.$$

Now

$$G_n(z) = z \left(1 + \frac{r_{2,1} r_{3,2} \mathbf{k}_1^T C \mathbf{k}_2 + O(z)}{r_{4,3} \mathbf{1}^T C \mathbf{k}_3 + O(z)} \right).$$

Thus, because of (5.5) and unless $\mathbf{k}_1^T C \mathbf{k}_2 = 0$, we have

$$G_n(z) = \frac{2}{3}z + O(z^2)$$

and the situation is actually *worse* than in the previous case!

So, let us proceed a step further, replacing (5.5) with

$$(5.6) \quad \mathbf{1}^T C \mathbf{k}_3 = \mathbf{k}_1^T C \mathbf{k}_2 = 0.$$

Another differentiation of $\mathbf{q}_1^T C \mathbf{q}_1 \equiv 0$ gives

$$(5.7) \quad \mathbf{1}^T C \mathbf{k}_4 + 4\mathbf{k}_1^T C \mathbf{k}_3 + 3\mathbf{k}_2^T C \mathbf{k}_2 = 0.$$

In the present case

$$\begin{aligned} G_n(z) &= z \left(1 + \frac{2r_{2,1} r_{4,3} \mathbf{k}_1^T C \mathbf{k}_3 + r_{3,2}^2 \mathbf{k}_2^T C \mathbf{k}_2 + O(z)}{2r_{5,4} \mathbf{1}^T C \mathbf{k}_4} \right) \\ &= z \left(1 + \frac{2\mathbf{k}_1^T C \mathbf{k}_3 + \mathbf{k}_2^T C \mathbf{k}_2 + O(z)}{\mathbf{1}^T C \mathbf{k}_4 + O(z)} \right). \end{aligned}$$

Thus, provided that $\mathbf{1}^T C \mathbf{k}_4 \neq 0$, $G_n(z) = O(z^2)$ if and only if

$$\mathbf{1}^T C \mathbf{k}_4 + 2\mathbf{k}_1^T C \mathbf{k}_3 + \mathbf{k}_2^T C \mathbf{k}_2 = 0.$$

Substituting the value of $\mathbf{1}^T C \mathbf{k}_4$ from (5.7) yields the conditions

$$(5.8) \quad \mathbf{1}^T C \mathbf{k}_4 \neq 0, \quad \mathbf{k}_1^T C \mathbf{k}_3 + \mathbf{k}_2^T C \mathbf{k}_2 = 0.$$

It is instructive to check (5.8) in \mathcal{C}_2^n for $n \in \{5, \dots, 7\}$. For $n = 5$ we have a one-dimensional space spanned by (3.8), and the latter gives

$$\mathbf{k}_1^T C \mathbf{k}_3 + \mathbf{k}_2^T C \mathbf{k}_2 = 2.$$

Likewise, for $n = 6$ we have

$$\mathbf{k}_1^T C \mathbf{k}_3 + \mathbf{k}_2^T C \mathbf{k}_2 = 4.$$

However, in the case $n = 7$ we have a two-dimensional space and

$$\begin{aligned} \mathbf{k}_1^T P_1 \mathbf{k}_3 + \mathbf{k}_2^T P_1 \mathbf{k}_2 &= 8, \\ \mathbf{k}_1^T P_2 \mathbf{k}_3 + \mathbf{k}_2^T P_2 \mathbf{k}_2 &= 2. \end{aligned}$$

Hence, the only possible choice of C (up to a nonzero multiplicative constant) which is consistent with the second condition in (5.8) is

$$P := P_1 - 4P_2 = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & -1 & -4 & 0 \\ 0 & 0 & 0 & 0 & 4 & 6 & -1 & 0 \\ 0 & 0 & 0 & -6 & -3 & 4 & 0 & 0 \\ 0 & 0 & 4 & -3 & -6 & 0 & 0 & 0 \\ 0 & -1 & 6 & 4 & 0 & 0 & 0 & 0 \\ 0 & -4 & -1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}.$$

Unfortunately, the first condition of (5.8) is violated, since $\mathbf{1}^T C \mathbf{k}_4 = 0$. This, in fact, is predictable – the function v for P is of the form

$$v(t) = v_1(t) - 4v_2(t) = (1-t)^6(1+t).$$

Thus, $d^\ell v(1)/dt^\ell = 0$, $\ell = 0, 1, \dots, 5$. But

$$\begin{aligned} v(1) &= \mathbf{1}^T C \mathbf{1}, \\ v'(1) &= \mathbf{1}^T C \mathbf{k}_1, \\ v''(1) &= \mathbf{1}^T C (\mathbf{k}_2 - \mathbf{k}_1), \\ v'''(1) &= \mathbf{1}^T C (\mathbf{k}_3 - 3\mathbf{k}_2 + 2\mathbf{k}_1) \end{aligned}$$

and so on. We conclude that $\mathbf{1}^T C \mathbf{k}_\ell = 0$, $\ell = 0, \dots, 5$. The general result can be phrased as a theorem.

THEOREM 5.1. *Suppose that*

$$f(z) = z + \sum_{\ell=2}^{\infty} \frac{1}{\ell!} \beta_\ell z^\ell$$

$$G(z) = \frac{\mathbf{u}^T C \mathbf{u}}{2\mathbf{1}^T C \mathbf{u}} \quad \text{where } C \in \mathcal{C}_p^{M_p} \quad \text{and } p \geq 1.$$

Then

$$G(z) = \alpha_p z + O(z^2) \quad \text{for } p \geq 1$$

where $\alpha_p \neq 0$ for $p = 1, 2, \dots, 5$. Furthermore, letting $L_p = J_1 + \dots + J_p$, it is true that $\sum_{j_1+j_2=2L_p} \mathbf{k}_{j_1}^T C_{M_p} \mathbf{k}_{j_2} \neq 0$ for $p \geq 6$ implies $\alpha_p \neq 0$.

Proof. Since $p \geq 1$, we have

$$\begin{aligned} \mathbf{1}^T C \mathbf{u} &= \sum_{\ell=3}^{\infty} \left(\sum_{j=2}^{\ell-1} r_{\ell,j} \mathbf{1}^T C \mathbf{k}_j \right) z^{\ell}, \\ \mathbf{u}^T C \mathbf{u} &= 2 \sum_{\ell=3}^{\infty} \left(\sum_{j=2}^{\ell-1} r_{\ell,j} \mathbf{1}^T C \mathbf{k}_j \right) z^{\ell+1} + \sum_{\ell_1=2}^{\infty} \sum_{\ell_2=2}^{\infty} \sum_{j_1=1}^{\ell_1-1} \sum_{j_2=1}^{\ell_2-1} r_{\ell_1,j_1} r_{\ell_2,j_2} \mathbf{k}_{j_1}^T C \mathbf{k}_{j_2} z^{\ell_1+\ell_2}. \end{aligned}$$

We will prove that, letting $\mathbf{k}_0 := \mathbf{1}$,

$$(5.9) \quad \mathbf{k}_i^T C_{M_p} \mathbf{k}_j = 0, \quad \text{for } 0 \leq i+j \leq 2L_p - 1.$$

Let

$$\begin{aligned} a_1(t, s) &= (t-s)(t-s); \\ a_p(t, s) &= a_{p-1}(t, s) \prod_{k=1, \gcd(k, p+1-k)=1}^{[p/2]} (t^k - s^{p+1-k})(t^{p+1-k} - s^k) \\ &= \prod_{k=1}^{[p/2]} \prod_{i=k, \gcd(i, k)=1}^{p+1-k} (t^i - s^k)(t^k - s^i). \end{aligned}$$

Then, since $a_p(t, s)$ has $2L_p$ factors of form $(t^k - s^l)$ and these factors are zero when $t = 1$ and $s = 1$,

$$\begin{aligned} \mathbf{k}_i^T C_{M_p} \mathbf{k}_j &= \frac{\partial}{\partial t} \left(t \frac{\partial}{\partial t} \left(t \cdots \frac{\partial}{\partial t} \left(t \frac{\partial}{\partial s} \left(s \frac{\partial}{\partial s} \left(s \cdots \frac{\partial}{\partial s} (a_p(t, s)) \cdots \right) \right) \right) \right) \right) \Big|_{t=1, s=1} \\ &= \left(\frac{\partial^{i+j}}{\partial t^i \partial s^j} a_p(t, s) + \sum_{k+l < i+j, 0 \leq k \leq i, 0 \leq l \leq j} \sigma_{k,l} \frac{\partial^{k+l}}{\partial k t \partial^l s} a_p(t, s) \right) \Big|_{t=1, s=1} \\ &= 0, \quad \text{for } 0 \leq i+j \leq 2L_p - 1, \end{aligned}$$

Furthermore,

$$\begin{aligned} \mathbf{1}^T C_{M_p} \mathbf{k}_{2L_p} &= \left[\frac{\partial^{2L_p}}{\partial t^{2L_p} \partial s} a_p(t, s) + \sum_{k+l < 2L_p} \sigma_{k,l} \frac{\partial^{k+l}}{\partial k t \partial^l s} a_p(t, s) \right] \Big|_{t=1, s=1} \\ &= (2L_p)! \prod_{k=1}^{[p/2]} \prod_{i=k, \gcd(i, k)=1}^{p+1-k} ik \neq 0. \end{aligned}$$

Consequently,

$$\mathbf{1}^T C_{M_p} \mathbf{u} = \sum_{l=2L_p+1}^{\infty} \left(\sum_{j=2L_p}^{l-1} r_{l,j} \mathbf{1}^T C_{M_p} \mathbf{k}_j \right) z^l$$

$$\begin{aligned}
&= \left(\frac{\beta_2}{2}\right)^{2L_p} \mathbf{1}^T C_{M_p} \mathbf{k}_{2L_p} z^{2L_p+1} + O(z^{2L_p+2}) \\
\mathbf{u}^T C_{M_p} \mathbf{u} &= 2 \sum_{l=2L_p+1}^{\infty} \left(\sum_{j=2L_p}^{l-1} r_{l,j} \mathbf{1}^T C_{M_p} \mathbf{k}_j \right) z^{l+1} \\
&\quad + \sum_{l_1+l_2>2L_p+1}^{\infty} \sum_{j_1=1}^{l_1-1} \sum_{j_2=2L_p-j_1}^{l_2-1} r_{l_1,j_1} r_{l_2,j_2} \mathbf{k}_{j_1}^T C_{M_p} \mathbf{k}_{j_2} z^{l_1+l_2} \\
&= 2r_{2L_p+1,2L_p} \mathbf{1}^T C_{M_p} \mathbf{k}_{2L_p} z^{2L_p+2} \\
&\quad + \sum_{j_1,j_2>0,j_1+j_2=2L_p} r_{j_1+1,j_1} r_{j_2+1,j_2} \mathbf{k}_{j_1}^T C_{M_p} \mathbf{k}_{j_2} z^{2L_p+2} + O(z^{2L_p+3}) \\
&= \left(\frac{\beta_2}{2}\right)^{2L_p} \sum_{j_1+j_2=2L_p} \mathbf{k}_{j_1}^T C_{M_p} \mathbf{k}_{j_2} z^{2L_p+2} + O(z^{2L_p+3}),
\end{aligned}$$

where $\mathbf{k}_0 = \mathbf{1}$. So we conclude

$$G(z) = \alpha_p z + O(z^2) \quad \text{for } p \geq 1,$$

where $\alpha_p \neq 0$ if $\sum_{j_1+j_2=2L_p} \mathbf{k}_{j_1}^T C_{M_p} \mathbf{k}_{j_2} \neq 0$. By direct calculation we can easily deduce that $\alpha_p \neq 0$ for $p = 1, 2, 3, 4, 5$. This completes the proof. \square

REFERENCES

- [1] C. BREZINSKI AND M. REDIVO ZAGLIA, *Extrapolation methods. Theory and Practice*, North-Holland, Amsterdam, 1993.
- [2] A. ISERLES, *Complex dynamics of convergence acceleration*, IMA J. of Numer. Anal., 11 (1991), pp. 205–240.